Diluted Generalized Random Energy Model

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We introduce a layered random spin model, equivalent to the Generalized Random Energy Model (GREM). In analogy with diluted spin systems, a diluted GREM (DGREM) is introduced. It can be applied to calculate approximately thermodynamic properties of spin glass models in low dimensions. For Edwards -Anderson model it gives correct critical dimension and 5% accuracy for ground state energy in 2d.

Derrida's Random Energy Model (REM) [1] was introduced as an archetype spin glass model. In recent years it is becoming more and more popular. It has been applied in many fields of physics, biology and even in information theory [2,3].

The REM is a mean-field model, like the Sherrington-Kirkpatrick model, but maximally simplified. But even after this simplification it appears to be a good approximation of some real systems.

The generalization of the REM (called Generalized Random Energy Model, GREM) was introduced in ref. [5]. It was used to solve approximately other spin glass systems [6,7]. Unfortunately, the accuracy to describe other SG systems was not much better than for the REM. In this work we introduce a diluted spin model which thermodynamically resembles GREM (in the case of large coordination number it is exactly equivalent to GREM), then construct some new model of energy configurations-DGREM. In some (practically important) cases our spin model is thermodynamically exactly equivalent to DGREM. There is another case of DGREM also, where we could not choose equivalent spin hamiltonian. Our new model is closer to realistic systems with a finite coordination number, than GREM.

Even the simpler diluted REM (DREM) [8,9] has proven to be a good approximation for models in low dimensions (d=1,2,3). This important fact was observed in [10], where by information-theoretical arguments (mathematically leading to a DREM) a percolation threshold was found.

We can estimate the ground state energy of the Edwards-Anderson model, using a DREM with the same number z of non-zero couplings [8,9]. It holds that on a hyper cubic lattice in d-dimensions $z = Nd$, where N is the number of spins. For another lattices one should replace d by the half of coordination number.

In the DREM one has N Ising spins interacting with each other in the z (randomly chosen from all the possible $C_N^p = \frac{N!}{p!(N-p)!}$) p-plets of Ising spins and quenched random couplings $\tau_{i_1,\cdots,i_p}$ having values ± 1.

The Hamiltonian reads

$$\mathcal{H} = - \sum_{(1\le i_1,\cdots<i_p\le N)=1}^{z} \tau_{i_1,\cdots,i_p}\sigma_{i_1}\cdots\sigma_{i_p} \qquad (1)$$

At high temperatures the system is in the para magnetic phase. There it has a free energy

$$\frac{F}{N} = -dT\ln\cosh\beta - T\ln 2 \qquad (2)$$

where $\beta = \frac{1}{T}$ Below the critical temperature $T_c = 1/\beta_c$ the system freezes in a spin-glass phase with internal energy

$$\frac{U}{N} = -d\tanh\beta_c \qquad (3)$$

and vanishing entropy

$$S = 0$$

Here $\tanh\beta_c = f(d)$ involves a function $f(x)$ defined by the implicit equation

$$\frac{1}{2}(1+f)\ln(1+f) + \frac{1}{2}(1-f)\ln(1-f)] = \frac{\ln 2}{x} \qquad (4)$$

Since the entropy is zero, we obtain for the ground state energy of the Edwards-Anderson model on a hyper cubic lattice in d dimensions

$$-\frac{E}{N} = f(d)d \qquad (5)$$

In 2d Esq. (5) gives $E \approx -1.5599$, which is close to result of Monte-Carlo simulation for the case of random ± 1 couplings [11] $\frac{E}{N} = -1.4015 \pm 0.0008$. This estimate by formula (3) was done by Derrida in his original work [1], long before the introduction of the DREM in reference [8].

Let us now construct some spin model, which has properties like the GREM. It is very important to have spin representation for GREM (for example- to construct temporal dynamics).
We consider a stacked system consisting of M planes with spin σ_i^k ordered along a "vertical" axis. In plane (layer) k there are N_k spins. The Hamiltonian is a sum of $M-1$ terms $H_{k,k+1}$ and one H_M. The last is as in eq. (1), with $N \to N_M, z \to z_M$ and all the interacting spins are from the M-th layer. For the $1 < k < M-1$ term $H_{k,k+1}$ describes interaction between spins of neibor layers k and $k+1$ through z_k p-plets of spins. In this case in any p-plet $\frac{p}{2}$ spins are chosen from the layer k and $\frac{p}{2}$ from the

layer $(k-1)$. Our z_k p-plets are chosen randomly from the all possible $[\frac{N!}{\frac{p}{2}!(N-\frac{p}{2})!}]^2$ ones. There are no "intra-plane" interactions terms (besides the spins of layer M) but only "inter-plane" interactions. So spins in the layer $1 < k < M$ interact with spins from the layers $k \pm 1$, the first layer interacts with the spins of second layer. We thus have the Hamiltonian

$$\mathcal{H} = - \sum_{(1\le i_1,\cdots<i_p\le N_M)}^{z_M} \tau_{i_1,\cdots,i_p}\sigma^M_{i_1}\cdots\sigma^M_{i_p} \qquad (6)$$

$$- \sum_{k=1}^{M-1} \sum_{(1\le i_1,\cdots<i_{\frac{p}{2}}\le N_{k-1}, 1\le j_1\cdots<j_{\frac{p}{2}}\le N_k)}^{z_k}$$

$$\tau_{i_1,\cdots,i_p}\sigma^{k-1}_{i_1}\cdots\sigma^{k-1}_{i_{\frac{p}{2}}}\sigma^k_{j_1}\cdots\sigma^k_{j_{\frac{p}{2}}}$$

Till now we considered spin model with some interaction among the spins. Let us now introduce some GREM like model. We consider some M level hierarchic tree. At first level there are 2_1^N branches. At second level every old branch fractures to 2^{N_2} new ones and so on. At the level M there are 2^N branches, where

$$N = \sum_{i=1,M}^{M} = N_i \qquad (7)$$

Energy configurations of our system are located on the ends of M-th level branches. On every branch of level i there are distributed random variables ϵ_i with the distribution

$$\rho_0(\epsilon_i, z_i) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \mathrm{d}k \exp[-k\epsilon_i + z_i \ln\cosh k] \qquad (8)$$

This is a distribution for a sum of z_k random ± 1 variables. So z_k resembles number of couplings in our diluted spin models. With any energy configuration are connected M branches. We define configuration energy as a sum (along the path on the tree, connected with chosen energy configuration) of these M variables ϵ_i. We see a usual picture of GREM, where random variable are distributed according to (7) instead of normal partition.

We can consider the case of large M with smooth distribution of z_k and N_k. In this case we can introduce continues variable $v = \frac{k}{M}$ between 0 and 1, labeling the level of planes and define distributions

$$z_k \equiv \mathrm{d}z = z\mathrm{d}v, \qquad N_k \equiv \mathrm{d}N = n'(v)\mathrm{d}v \qquad \mathrm{d}v = \frac{1}{M} \quad (9)$$

where $n(v)$ is a given function (entropy in bits-s). The variable v ($0 < v < 1$) parameterizes the level of the hierarchical tree and z is a parameter (for our spin system z is a total number of couplings and parameter v labeling the level of planes).
Of course, our function $n(v)$ should be monotonic. Total number of energy configurations is $2^{n(0)}$ and

$$n(0) = N \qquad (10)$$

We have, that 2^N energy levels E of our hierarchic model are distributed by partition

$$\rho(E) = \rho_0(E, z) \qquad (11)$$

If two configurations (in our GREM like model) meet at level of hierarchy v, they have zv common random variables. The energy difference between two configurations is related to $z(1-v)$ non-common random variables. Therefore the distribution function of two energies E_1, E_2 reads

$$\rho_2(E_1 - E_2) = \rho_0((E_1 - E_2), 2z(1-v))\exp(\ln 2 n(v)) \qquad (12)$$

At high temperatures our system is in the para magnetic phase. The free energy is given by eq. (2). When we decrease the temperature, two situations are possible: First, $\frac{dz}{dN} \equiv \frac{z}{n'(v)}$ decreases monotonically with v; second, it has a local maxim.
In the first case the system has no sharp phase transition but it freezes gradually. At temperature $T = \frac{1}{\beta}$ all level with $0 \le v \le v_f(T)$ are frozen; they are in the spin glass phase. The levels with $v_f < v \le 1$ are in the paramagnetic phase. v_f is defined as the solution $v_f = v$ of equation

$$\tanh\beta = f(\frac{z}{n'(v)}) \qquad (13)$$

Using this relationship between β and v we can later use functions $v(\beta)$ and $\beta(v)$. For every finite β the value of $v(\beta)$ lies between zero and unity. When $T \to \infty$, $v(\beta) \to 0$ and when $T \to 0$,$v(\beta) \to v_0 > 0$. So even in this limit some part of spins stay in their para magnetic phase. Let us point out that this partial freezing only is possible in the Diluted GREM, and not in the original GREM. For the free energy we obtain (there is no factor N in it):

$$-\beta F = \quad z(1-v(\beta))\ln\cosh\beta + n(v(\beta))\ln 2 + z\beta\int_0^{v(\beta)} \mathrm{d}v_1 f(\frac{z}{n'(v_1)}) \qquad (14)$$

The first two terms in the right hand side describes the para magnetic fraction of free energy ($n(v(\beta))\ln 2$ just is the entropy), while the last one desrcibe the fraction of spins frozen in a glassy configuration (it resembles equation (3) with $\frac{z}{f'(v_1)}$ instead of d).
In the second case (function $n'(v)$ is not monotonic) the

system has a sharp first order phase transition at a finite temperature T_2. Below T_2 freezing occurs drastically for all levels $v < v_2$, where $v_2 \equiv v(\beta_2)$ is defined by the equation

$$n'(v_2) = N - n(v_2) \tag{15}$$

We used the fact that $n(0) = N$. The transition temperature $T_2 = \frac{1}{\beta_2}$ follows from

$$\tanh(\beta_2) = f(\frac{z}{n'(v_2)}) \tag{16}$$

For temperatures $T < T_2$ the free energy reads

$$-\frac{\beta F}{N} = \quad z(1-v(\beta))\ln\cosh\beta + n(v(\beta))\ln 2 + zv(\beta_2)\beta f(\frac{z}{n'(v_2)}) + z\beta\int_{v_2}^{v(\beta)} \mathrm{d}v_1 f(\frac{z}{n'(v_1)}) \tag{17}$$

Protein folding probably corresponds to this case. To construct the spin Hamiltonian by means of chain of subsystems for this case is still an open problem.

Let us now consider a possible approximation to the Edwards-Anderson model, following the idea's presented in ref. [6]. In the d-dimensional case our 2^N energy levels E are distributed according to the law

$$\rho(\epsilon) = \rho_0(\epsilon, Nd) \tag{18}$$

with ρ_0 defined in eq. (8) Comparing with (11) one immediately notices that this is exactly equivalent to a DGREM with the choice $E = \epsilon$, $z = Nd$. Let us now consider the distribution of $\epsilon_1 - \epsilon_2$. Following the arguments presented in reference [6], we find that

$$\rho_2(\epsilon_1 - \epsilon_2) = \rho_0(\frac{\epsilon_1 - \epsilon_2}{2}, Nd(1-y))\exp Ns(-dN(2y-1)) \tag{19}$$

where $s(E)$ is the entropy of a ferromagnetic system on the same lattice with internal energy equal E. Physical meaning of the last equation is transparent [6]. If we consider partition of two spin configurations, then one of them could be chosen (due to gauge invariance) as ordered configuration with $\sigma_i = 1$ for all spins. In this case energy of first configuration equals to sum of dN random $\pm$ couplings and energy of second - sum of the Ndy random variables with the same sign, and $Nd(1-y)$ with the opposite sign. Distribution of second configurations by y just equals to number of configurations with energy $E = -(2y-1)Nd$ in ferromagnetic model. For the last in thermodynamic limit we have expression $\exp Ns(-dN(2y-1)$. Unfortunately it differs from eq. (12). So it is impossible to choose a DGREM with the given correlation functions for E and $E_1 - E_2$. We can consider an approximation. One choice is to take the exact expression for $\rho(\epsilon)$ and make an approximation for $\rho(\epsilon_1 - \epsilon_2)$.

$$z = Nd, \quad \epsilon = E, \quad v = 2y - 1, \quad n(v) = \frac{Ns(-vdN)}{\ln 2} \tag{20}$$

We see, that variable v, givimg distribution for the number of couplings among the hierarchy corresponds to energy per bond in ferromagnetic model. We can remember from definition of temperature

$$\frac{\mathrm{d}s}{\mathrm{d}E} = \frac{1}{\tau} \equiv \beta \tag{21}$$

At given $\tilde{\beta}_1$ we can define corresponding v_1 as minus energy per bond for ferromagnetic model at temperature $\frac{1}{\tilde{\beta}_1}$.

$$v_1 = -\frac{E(\tilde{\beta}_1)}{Nd} \tag{22}$$

We obtain for the free energy

$$-\frac{\beta F}{Nd} = (1-v(\beta))\ln\cosh\beta + s(v(\beta)) + \beta\int_0^{v(\beta)} \mathrm{d}v_1 f(\frac{\ln 2}{\tilde{\beta}}) \tag{23}$$

Integrating by parts in the last term we get

$$-\frac{\beta F}{Nd} = (1-v(\beta))\ln\cosh\beta + s(v(\beta)) - \beta\int_0^{\tilde{\beta}} \mathrm{d}\tilde{\beta}_1 \frac{2v_1(\tilde{\beta}_1)}{\ln\frac{1+y}{1-y}} + v(\beta)\beta y(\tilde{\beta}) \tag{24}$$

where y as a function of $\tilde{\beta}_1$ is defined from the equation

$$y = f(\frac{\ln 2}{\tilde{\beta}_1}) \tag{25}$$

function $v(\beta)$ is defined from (13), and $v_1(\tilde{\beta}_1)$ is minus energy per bond in ferromagnetic model at temperature $\tilde{\beta}_1$. In the equation (24) value of the $\tilde{\beta}$ is connected with the given β via the equation

$$\tanh(\beta) = f(\frac{\ln 2}{\tilde{\beta}}) \tag{26}$$

In the limit of zero temperature **this reduces to**

$$-\frac{\beta F}{N} = d[1 - \frac{2}{d}\int_0^{\ln 2} \frac{\mathrm{d}\tilde{\beta}_1 E(\tilde{\beta}_1)}{\ln\frac{1+y(\tilde{\beta}_1)}{1-y(\tilde{\beta}_1)}}] \tag{27}$$

He $E(\tilde{\beta}) = |U|$ is minus the energy in the ferromagnetic model, $y(\tilde{\beta})$ is defined from (25) and function $f(x)$ from the (4). If the ferromagnetic system has a phase transition at $\tilde{\beta}_c$, then the DGREM has one at β_c **determined by**

$$\beta_c = \frac{1}{2}\ln\frac{1+f(\frac{\ln 2}{\tilde{\beta}_c})}{1-f(\frac{\ln 2}{\tilde{\beta}_c})} \tag{28}$$

This equation has solution only if

$$\ln 2 \, / \tilde{\beta}_c > 1 \tag{29}$$

As for 2d Ising model $\ln 2 < \tilde{\beta}_c$, it follows that for the 2d Edwards-Anderson model there **does not occur a phase transition at a finite temperature.** is not any phase transition at finite temperatures. **A** calculation of **the ground state** energy in this case using (27) gives $E = -1.4763$. More generally, for the case of other models one can use numerical data for **the** ferromagnetic system to calculate **the** ground state energy of **the** corresponding SG model on the same lattice.
In the case of 3d Ising model we have for transition point $\beta_c = 0.2216$. In this case inequality (29) is satisfied. So our method gives as critical dimension for EA model $d = 3$.
In conclusion, we have suggested a **a diluted version of the generalized random energy model** and applied to find a simple approximation to the ground state energy of disordered systems and definition of critical dimensions.

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